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Molecular simulation studies of morphology in blends of conjugated polymers and fullerene derivatives for organic photovoltaic applications ERIC JANKOWSKI, HILARY MARSH, ARTHI JAYARAMAN, University of Colorado at Boulder — The device efficiency of organic solar cells is dependent on the microstructure of the active layer, which is typically a mixture of conjugated polymer electron donor molecules and fullerene based acceptor molecules. Active layer morphology can be tuned by choosing these acceptor and donor components that self-assemble into thermodynamically stable structures and by choosing processing conditions that facilitate the formation of equilibrium structures or that "trap" the active layer in an optimal metastable configuration. We present the results of molecular dynamics studies of model conjugated polymers and fullerene derivatives performed on GPUs. We show that the ordered structures that are self-assembled from initially disordered configurations depend strongly upon the strength of the attractions between acceptor and donor molecules, the relative amounts of each component, and the architecture of the donor molecules. Further we quantify the relaxation times and suggest processing strategies for obtaining optimal morphologies for charge transport.

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